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Subsection 1448A/PTO

INFORMATION DISCLOSURE STATEMENT BY APPLICANT

(use as many sheets as necessary)

Sheet 1

of

4

Complete if Known

Application Number	10/053,354
Filing Date	November 2, 2001
First Named Inventor	Rosenthal, Dan E.
Art Unit	2123
Examiner Name	Unassigned
Attorney Docket Number	020910-000210US

U.S. PATENT DOCUMENTS

Examiner	Cite No. ¹	Document Number Number Kind Code ² (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear
CVL	AA	US 6,512,997	1/28/2003	Padilla, et al.	
CVL	AB	US 6,253,166	6/26/2001	Whitmore, et al.	
CVL	AC	US 6,185,506	2/6/2001	Cramer, III, et al.	
CVL	AD	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	
CVL	AE	US 6,150,179	11/21/2000	Went	
CVL	AF	US 6,125,235	9/26/2000	Padilla, et al.	
CVL	AG	US 6,081,766	6/27/2000	Chapman, et al.	
CVL	AH	US 6,014,449	1/11/2000	Jacobs, et al.	
CVL	AI	US 5,799,312	8/25/1998	Rigoutsos	
CVL	AJ	US 5,787,279	7/28/1998	Rigoutsos	
CVL	AK	US 5,777,889	7/7/1998	Mohanty, et al.	
CVL	AL	US 5,752,019	5/12/1998	Rigoutsos, et al.	
CVL	AM	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
CVL	AN	US 5,625,575	4/29/1997	Goyal, et al.	
CVL	AO	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
CVL	AP	US 5,307,287	4/26/1994	Cramer, III, et al.	

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FOREIGN PATENT DOCUMENTS

Examiner Initials*	Cite No. ¹	Foreign Patent Document			Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	T ⁶
		Country Code ³	Number ⁴	Kind Code ⁵ (if known)				
CVL	AQ	WO	02/073334	A2	07-26-1990	Padilla, et al.		<input type="checkbox"/>
CVL	AR	WO	01/67310	A1	12-12-1991	Smith, et al.		<input type="checkbox"/>
CVL	AS	WO	96/24902	A1	04-01-1993	Wertz		<input type="checkbox"/>

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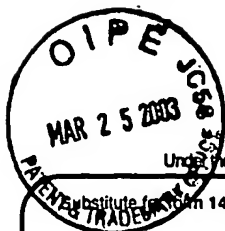
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6/27/05

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Sheet 2	of 4	Attorney Docket Number	020910-000210US

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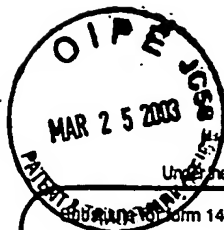
OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS			
Examiner Initials *	Cite No. ¹	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T ²
CVL	AT	ASCHER, et al., <u>Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations</u> , 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	
CVL	AU	BARAFF, et al., " <u>Large steps in cloth simulation</u> ", 1998, <u>Computer Graphics Proceedings SIGGRAPH 98</u> (Orlando, July 19-24) p43.pdf	
CVL	AV	BARTH, et al., " <u>A separating framework for increasing the timestep in molecular dynamics</u> " in <u>Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3</u> , 1997, pgs. 97-121, Kluwer Academic Dordrecht, The Netherlands.	
CVL	AW	BERENDSEN, " <u>Molecular Dynamics Simulations: The Limits and Beyond</u> " in <u>Computational Molecular Dynamics: Challenges, Methods, Ideas</u> , 1999, pgs. 3-36, Springer-Verlag, Germany.	
CVL	AX	BISCHOF, et al., <u>ADIFOR 2.0 Users' Guide</u> , 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
CVL	AY	BRENAN, et al., <u>Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations</u> , 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
CVL	AZ	BUTCHER, " <u>Towards efficient implementation of singly-implicit methods</u> ", 1988, <u>AMC Transactions of Mathematical Software</u> 14:68-75.	
CVL	BA	BYSTROFF, " <u>An alternative derivation of the equations of motion in torsion space for a branched linear chain</u> ", 2001, <u>Protein Engineering</u> 14:825-828.	
CVL	BB	COLEMAN, et al., " <u>The efficient computation of sparse Jacobian matrices using automatic differentiation</u> ", 1996, <u>Cornell Theory Center Technical Report CTC95TR225</u> .	
CVL	BC	EICHBERGER, et al., " <u>The benefits of parallel multibody simulation</u> ", 1994, <u>International Journal for Numerical Methods in Engineering</u> , 37:1557-1572.	
CVL	BD	GOLUB, et al., " <u>The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate</u> ", 1973, <u>SIAM J. Numer. Anal.</u> 10:413.	
CVL	BE	HAIRER, et al., <u>Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems</u> , 2nd ed., 1996, Springer-Verlag, Germany.	
CVL	BF	HE, et al., " <u>Macromolecular conformational dynamics in torsional angle space</u> ", 1998, <u>Journal of Chemical Physics</u> 108:271.	
CVL	BG	HOLLARS, et al., <u>SD/FAST User's Manual, Version B.2</u> , 1994, Symbolic Dynamics, California.	

Examiner Signature		Date Considered	4/27/05
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		Filing Date	November 2, 2001		
		First Named Inventor	Rosenthal, Dan E.		
		Art Unit	2123		
		Examiner Name	Unassigned		
Sheet	3	of	4	Attorney Docket Number	020910-000210US

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OTHER PRIOR ART – NON PATENT LITERATURE DOCUMENTS			
Examiner Initials *	Cite No. ¹	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T ²
CVL	BH	IZAGUIRRE, et al., "Longer Time Steps for Molecular Dynamics", 1999, <u>J.Chem.Phys.</u> 110:9853.	
CVL	BI	KANE, <u>Dynamics</u> , 3rd ed., 1978, Stanford University, Stanford, California.	
CVL	BJ	LEACH, <u>Molecular Modelling Principles and Applications</u> , 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.	
CVL	BK	MARTINS, et al., "An automated method for sensitivity analysis using complex variables", 2000, <u>American Institute of Aeronautics and Astronautics</u> , 2000-0689 p1	
CVL	BL	MOROKUMA, et al., "Model studies of the structures, reactivities, and reaction mechanisms of metalloenzymes", 2001, <u>IBM J. Res. & Dev.</u> 45(3/4):367-395.	
CVL	BM	NORSETT, et al., "Embedded SDIRK-methods of basic order three", 1984, <u>BIT</u> 24:634-646.	
CVL	BN	PONDER, <u>TINKER User's Guide, Version 3.8</u> , October 2000, Washington University, St. Louis, MO.	
CVL	BO	RAPAPORT, <u>The Art of Molecular Dynamics Simulation</u> , 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.	
CVL	BP	SCHLICK, "Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation", 1997, <u>Annu. Rev. Biophys. Biomol. Struct.</u> , 26:181-222.	
CVL	BQ	SCHLICK, "Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations" in <u>Computational Molecular Dynamics: Challenges, Methods, Ideas</u> , 1999, pgs. 227-262, Springer-Verlag, Germany.	
CVL	BR	SCHLICK, <u>Molecular Modeling and Simulation - An Interdisciplinary Guide</u> , 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlag, Germany.	
CVL	BS	SHAMPINE, "Implementation of implicit formulas for the solution of ODEs", 1980, <u>SIAM J. Sci. Stat. Comput.</u> 1:103-118.	
CVL	BT	VERLET, "Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules", 1967, <u>Physical Review</u> , 159(1):98-103.	
CVL	BU	VON SCHWERIN, <u>Multibody System Simulation</u> , 1999, Springer-Verlag, Germany.	

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		Filing Date	November 2, 2001
		First Named Inventor	Rosenthal, Dan E.
		Art Unit	2123
		Examiner Name	Unassigned
Sheet 4 of 4	Attorney Docket Number	020910-000210US	

OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS			
Examiner Initials *	Cite No. ¹	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T ²
CVL	BV	WU, et al., "Constraint dynamics algorithm for simulation of semiflexible macromolecules", 1998, <u>Journal of Computational Chemistry</u> 19:1555-1566	
CVL	BW	YEN, et al., "On the numerical solution of constrained multibody dynamic systems", 1994, <u>University of Minnesota AHPCRC</u> 94-038.	

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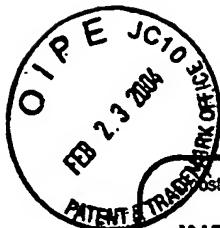
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CVL		ABAGYAN, et al., "New Methodology for Computer-Aided Modelling of Biomolecular Structure and Dynamics 2. Local Deformation Cycles", 1989, <u>Journal of Biomolecular Structure & Dynamics</u> 6(4):833-845.	
CVL		GIBSON, et al., "Variable Step Molecular Dynamics: An Exploratory Technique for Peptides with Fixed Geometry", 1990, <u>Journal of Computational Chemistry</u> 11(4):468-486.	
CVL		JAIN, et al., "Linearization of Manipulator Dynamics Using Spatial Operators", 1993, <u>IEEE Transactions on Systems, Man and Cybernetics</u> 23(1):239-248.	
CVL		LUDOVICE, et al., "Molecular dynamics of geometrically constrained polymer systems in generalized coordinates: Basic formalism", 1991, <u>Computational Polymer Science</u> 1:69-79.	
CVL		MAZUR, et al., "New Methodology for Computer-Aided Modelling of Biomolecular Structure and Dynamics 1. Non-Cyclic Structures", 1989, <u>Journal of Biomolecular Structure & Dynamics</u> 6(4):815-832.	
CVL		PESKIN, ET AL., "Molecular Dynamics by the Backward-Euler Method", 1989, <u>Communications on Pure and Applied Mathematics XLII</u> :1011-1031.	
CVL		ROSENTHAL, et al., "High Performance Multibody Simulations via Symbolic Equation Manipulation and Kane's Method", 1986, <u>The Journal of the Astronautical Sciences</u> , 34(3):223-239.	
CVL		ROSENTHAL, "An Order n Formulation for Robotic Systems", 1990, <u>The Journal of the Astronautical Sciences</u> , 38(4):511-529.	
CVL		ROSENTHAL, "Engineers Notes: Triangulation of Equations of Motion for Robotic Systems", 1988, <u>The Journal of Guidance</u> , 11(3):278-281.	
CVL		SCHLICK, et al., "A molecular dynamics simulation of a water droplet by the implicit Euler/Langevin scheme", 1991, <u>J. Chem. Phys.</u> , 94(3):2118-2129.	
CVL		ZHANG, et al., "The Langevin/implicit-Euler/normal-mode scheme for molecular dynamics at large timesteps", 1994, <u>J. Chem. Phys.</u> , 101(6):4995-5012.	

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